



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2025 – 08:39 AM EDT

PDB ID : 3SVR  
Title : Crystal structure of mkate mutant S158A/S143C at pH 7.5  
Authors : Wang, Q.; Byrnes, L.; Sondermann, H.  
Deposited on : 2011-07-12  
Resolution : 1.91 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

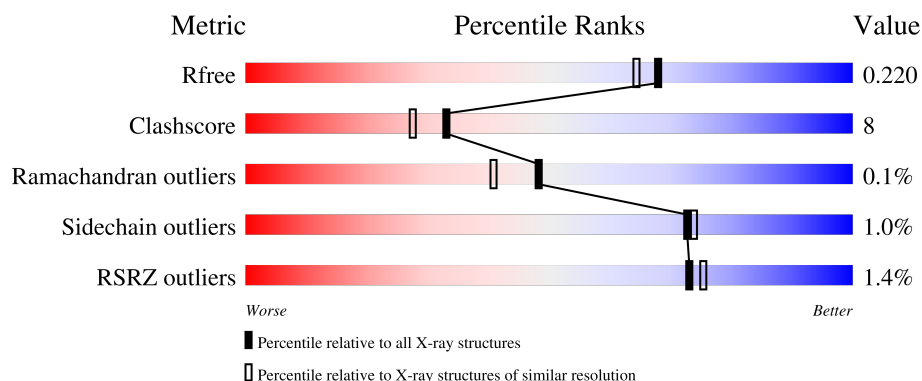
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 1.91 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	233	
1	B	233	
1	C	233	
1	D	233	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	NRQ	A	63[A]	-	-	X	-
1	NRQ	C	63[A]	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8095 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called mkate S158A/S143C.

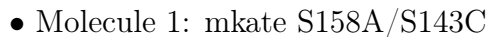
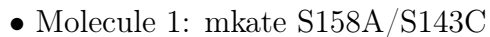
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	2	0
			1789	1141	301	331	16			
1	B	229	Total	C	N	O	S	0	7	0
			1868	1190	316	345	17			
1	C	228	Total	C	N	O	S	0	8	0
			1862	1184	316	346	16			
1	D	225	Total	C	N	O	S	0	2	0
			1811	1153	305	337	16			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	201	Total	O	0	0
			201	201		
2	B	219	Total	O	0	0
			219	219		
2	C	191	Total	O	0	0
			191	191		
2	D	154	Total	O	0	0
			154	154		



- Molecule 1: mkate S158A/S143C



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.31Å 161.31Å 75.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.33 – 1.91 40.33 – 1.91	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.33-1.91) 97.7 (40.33-1.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.180 , 0.227 0.174 , 0.220	Depositor DCC
$R_{free}$ test set	3736 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NRQ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.40	0/1784	0.58	0/2405
1	B	0.39	0/1880	0.57	0/2532
1	C	0.38	0/1878	0.55	0/2535
1	D	0.38	0/1807	0.54	0/2438
All	All	0.39	0/7349	0.56	0/9910

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1789	0	1758	30	0
1	B	1868	0	1841	28	0
1	C	1862	0	1818	33	0
1	D	1811	0	1773	26	0
2	A	201	0	0	4	0
2	B	219	0	0	8	0
2	C	191	0	0	6	0
2	D	154	0	0	3	0
All	All	8095	0	7190	112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 112 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ASP:OD2	2:B:757:HOH:O	1.83	0.95
1:B:20:ASN:O	2:B:761:HOH:O	1.85	0.94
1:C:63[B]:NRQ:HD2	1:C:63[B]:NRQ:O2	1.66	0.94
1:D:159:ASP:OD1	2:D:417:HOH:O	1.89	0.89
1:C:212:GLU:OE1	2:C:411:HOH:O	1.92	0.87

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/233 (92%)	213 (99%)	2 (1%)	0	100	100
1	B	229/233 (98%)	226 (99%)	3 (1%)	0	100	100
1	C	230/233 (99%)	224 (97%)	5 (2%)	1 (0%)	30	22
1	D	221/233 (95%)	218 (99%)	3 (1%)	0	100	100
All	All	895/932 (96%)	881 (98%)	13 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	20	ASN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar



resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/195 (97%)	190 (100%)	0	100	100
1	B	199/195 (102%)	195 (98%)	4 (2%)	50	47
1	C	198/195 (102%)	196 (99%)	2 (1%)	73	74
1	D	191/195 (98%)	189 (99%)	2 (1%)	73	74
All	All	778/780 (100%)	770 (99%)	8 (1%)	73	74

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	223	ASP
1	D	29	GLU
1	C	41	MET
1	B	223	ASP
1	C	223	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	214	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	NRQ	C	63[A]	1	24,24,25	5.37	8 (33%)	24,32,34	2.72	6 (25%)
1	NRQ	D	63[A]	1	24,24,25	5.33	8 (33%)	24,32,34	3.21	5 (20%)
1	NRQ	A	63[B]	1	24,24,25	5.52	9 (37%)	24,32,34	2.97	7 (29%)
1	NRQ	B	63[A]	1	24,24,25	5.25	8 (33%)	24,32,34	3.03	7 (29%)
1	NRQ	C	63[B]	1	24,24,25	5.56	8 (33%)	24,32,34	3.38	9 (37%)
1	NRQ	B	63[B]	1	24,24,25	5.55	8 (33%)	24,32,34	3.59	10 (41%)
1	NRQ	D	63[B]	1	24,24,25	5.32	8 (33%)	24,32,34	3.14	8 (33%)
1	NRQ	A	63[A]	1	24,24,25	5.42	9 (37%)	24,32,34	2.52	6 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NRQ	C	63[A]	1	-	2/9/31/32	0/2/2/2
1	NRQ	D	63[A]	1	-	1/9/31/32	0/2/2/2
1	NRQ	A	63[B]	1	-	4/9/31/32	0/2/2/2
1	NRQ	B	63[A]	1	-	2/9/31/32	0/2/2/2
1	NRQ	C	63[B]	1	-	4/9/31/32	0/2/2/2
1	NRQ	B	63[B]	1	-	5/9/31/32	0/2/2/2
1	NRQ	D	63[B]	1	-	2/9/31/32	0/2/2/2
1	NRQ	A	63[A]	1	-	2/9/31/32	0/2/2/2

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63[A]	NRQ	CB2-CA2	20.03	1.54	1.35
1	B	63[B]	NRQ	CB2-CA2	19.98	1.54	1.35
1	C	63[B]	NRQ	CB2-CA2	19.86	1.54	1.35
1	A	63[B]	NRQ	CB2-CA2	19.68	1.54	1.35
1	C	63[A]	NRQ	CB2-CA2	19.20	1.53	1.35

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63[A]	NRQ	O2-C2-CA2	-9.47	124.98	131.02
1	B	63[A]	NRQ	O2-C2-CA2	-9.14	125.19	131.02
1	A	63[B]	NRQ	O2-C2-CA2	-8.67	125.49	131.02

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63[A]	NRQ	CG2-CB2-CA2	-8.57	119.67	129.87
1	B	63[B]	NRQ	CB2-CA2-C2	8.08	132.15	122.36

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63[A]	NRQ	CA1-CB1-CG1-SD
1	A	63[B]	NRQ	N2-CA2-CB2-CG2
1	A	63[B]	NRQ	C2-CA2-CB2-CG2
1	B	63[A]	NRQ	CA1-CB1-CG1-SD
1	B	63[B]	NRQ	N2-CA2-CB2-CG2

There are no ring outliers.

8 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	63[A]	NRQ	10	0
1	D	63[A]	NRQ	6	0
1	A	63[B]	NRQ	3	0
1	B	63[A]	NRQ	6	0
1	C	63[B]	NRQ	3	0
1	B	63[B]	NRQ	4	0
1	D	63[B]	NRQ	3	0
1	A	63[A]	NRQ	10	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	220/233 (94%)	-0.28	0 <b>100</b> <b>100</b>	14, 24, 41, 60	1 (0%)
1	B	228/233 (97%)	-0.25	4 (1%) 67 70	13, 24, 38, 56	6 (2%)
1	C	227/233 (97%)	-0.17	6 (2%) 57 59	15, 26, 40, 47	7 (3%)
1	D	224/233 (96%)	-0.08	3 (1%) 74 76	15, 28, 44, 60	1 (0%)
All	All	899/932 (96%)	-0.20	13 (1%) 73 75	13, 26, 41, 60	15 (1%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	152	GLY	3.0
1	C	3	ALA	2.8
1	D	2	SER	2.7
1	C	2	SER	2.6
1	D	3	ALA	2.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	NRQ	A	63[A]	23/24	0.93	0.08	17,22,24,31	23
1	NRQ	A	63[B]	23/24	0.93	0.08	15,21,24,30	23
1	NRQ	D	63[A]	23/24	0.94	0.08	21,23,27,32	23
1	NRQ	D	63[B]	23/24	0.94	0.08	20,24,27,29	23
1	NRQ	C	63[A]	23/24	0.95	0.07	18,22,25,32	23
1	NRQ	C	63[B]	23/24	0.95	0.07	18,21,24,29	23
1	NRQ	B	63[A]	23/24	0.95	0.08	17,20,25,30	23

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	NRQ	B	63[B]	23/24	0.95	0.08	18,20,24,29	23

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.